

Density functional theory of a trapped Bose gas with tunable scattering length: from weak-coupling to unitarity

Maurizio Rossi¹, Francesco Ancilotto^{1,2}, Luca Salasnich^{1,3}, Flavio Toigo^{1,2}

Dipartimento di Fisica e Astronomia "Galileo Galilei" and CNISM,

Università di Padova, via Marzolo 8, 35122 Padova, Italy

CNR-IOM Democritos, via Bonomea, 265 - 34136 Trieste, Italy

CNR-INO, via Nello Carrara, 1 - 50019 Sesto Fiorentino, Italy

We study an interacting Bose gas at $T=0$ under isotropic harmonic confinement within Density Functional Theory in the Local Density approximation. The energy density functional, which spans the whole range of positive scattering lengths up to the unitary regime (infinite scattering length), is obtained by fitting the recently calculated Monte Carlo bulk equation of state [Phys. Rev. A **89**, 041602(R) (2014)]. We compare the density profiles of the trapped gas with those obtained by MC calculations. We solve the time-dependent Density Functional equation to study the effect of increasing values of the interaction strength on the frequencies of monopole and quadrupole oscillations of the trapped gas. We find that the monopole breathing mode shows a non-monotonous behavior as a function of the scattering length. We also consider the damping effect of three-body losses on such modes.

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Motivated by promising experimental observations [1–4], in a very recent paper [5] we have investigated the zero-temperature properties of a dilute homogeneous Bose gas by tuning the interaction strength of the two-body potential to achieve arbitrary positive values of the s-wave scattering length a . In that paper [5] we have computed by Monte Carlo (MC) quadrature the energy per particle and the condensate fraction of the system by using a Jastrow ansatz for the many-body wave function which avoids the formation of the self-bound clusters present in the ground-state and describes instead a (metastable) gaseous state with uniform density.

Here we set up a reliable energy density functional (DF) for bosons under external confinement by fitting the MC equation of state of the bulk system [5].

The Kohn-Sham formulation[6] of time-dependent Density Functional Theory (TDDFT)[7] for an inhomogeneous system of interacting bosons at $T=0$ (with local number density $n(\mathbf{r})$ and mass M) is described, within the Local Density Approximation, by the equation:

$$i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = \left[-\frac{\hbar^2 \nabla^2}{2M} + U(\mathbf{r}) + \frac{\partial(n\varepsilon_a)}{\partial n} \right] \Psi(\mathbf{r}, t) \quad (1)$$

where $|\Psi(\mathbf{r})|^2 = n(\mathbf{r})$ and $\varepsilon_a(n(\mathbf{r}))$ is the energy per atom of a *homogeneous* system with density equal to the local density. Here $U(\mathbf{r})$ describes the external confinement, which we assume to be an isotropic harmonic potential, $U(\mathbf{r}) = \frac{1}{2}M\omega_H^2(x^2 + y^2 + z^2)$. The associated total energy functional is

$$E = \int d^3\mathbf{r} \left\{ \frac{\hbar^2}{2M} |\nabla \Psi(\mathbf{r})|^2 + n(\mathbf{r})\varepsilon_a(n(\mathbf{r})) + n(\mathbf{r})U(\mathbf{r}) \right\}. \quad (2)$$

As previously discussed, the values of $\varepsilon_a(n)$ have been recently computed with a MC approach [5] for a wide range of (positive) values of the scattering length a characterizing the interparticle interaction. In the weakly interacting regime ($x \equiv a/r_0 \ll 1$, where $r_0 = (3/(4\pi n))^{1/3}$ is the average distance between bosons) the MC results for $\varepsilon_a(n)$ are very close to $\varepsilon_{\text{LHY}}(n)$, the universal Bogoliubov prediction [8] as corrected by Lee, Huang and Yang (LHY) [9]. In the strong-coupling regime ($x \gg 1$), instead, MC data reach a plateau and, in the unitary limit ($a \rightarrow \infty$), a finite and positive energy per particle is found, $E/N = 0.70 \varepsilon_B(n)$, where $\varepsilon_B(n) = \frac{\hbar^2}{2M}(6\pi^2 n)^{2/3}$.

The equation of state [5] from such MC calculation can be well interpolated as:

$$\frac{\varepsilon_a(n)}{\varepsilon_B(n)} = \begin{cases} f_{\text{LHY}}(x) + a_3 x^3 & \text{for } x < 0.3 \\ c_7 x^7 + c_6 x^6 + c_5 x^5 + c_4 x^4 + c_3 x^3 + c_2 x^2 + c_1 x + c_0 & \text{for } 0.3 < x < 0.5 \\ b_0 + b_1 \tanh(b_2/x - 1) & \text{for } x > 0.5 \end{cases} \quad (3)$$

with $a_3 = 0.21$, $b_0 = 0.45$, $b_1 = -0.33$, $b_2 = 0.54$, $c_0 = 4.75$, $c_1 = -99.72$, $c_2 = 890.68$, $c_3 = -4309.56$, $c_4 = 12268.41$, $c_5 = -20488.00$, $c_6 = 18568.27$ and $c_7 = -7052.20$ [10]. In (3), $f_{\text{LHY}}(x) = \left(\frac{4}{3\pi^2}\right)^{1/3} x \left[1 + \frac{128}{15\sqrt{\pi}} \sqrt{\frac{3}{4\pi}} x^{3/2}\right]$ is the LHY correction to the Bogoliubov prediction.

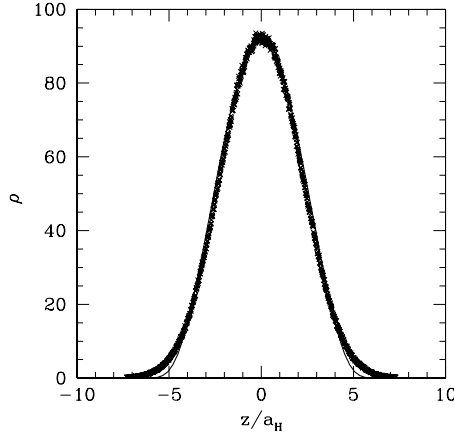


FIG. 1: Integrated density profile $\rho(z)$ for $N = 500$ bosons with $a = 10^4 a_0$ under isotropic harmonic confinement. Solid line: DFT results; points: MC results. Here $a_H \equiv \sqrt{\hbar/(M\omega_H)}$.

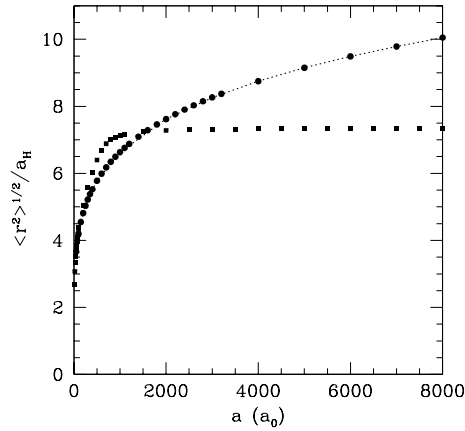


FIG. 2: Average radius of the trapped gas as a function of a . Squares: DFT results; dots: GPE results with the same value of a . The dotted line shows the GPE result in the TF limit, where $\langle r^2 \rangle^{1/2} \propto a^{1/5}$.

Notice that in the deep weak-coupling regime Eq. (1) reduces to the familiar Gross-Pitaevskii equation (GPE) [11] since $\varepsilon_a(n) = \mathcal{E}_{\text{GPE}}(n, a) \equiv 2\pi\hbar^2 a n^2 / M$.

In Fig.1 we show the ground-state integrated density profile $\rho(z) = \int dx dy n(x, y, z)$ for $N = 500$ bosons and $a = 10^4$ (in units of the Bohr radius a_0) obtained by numerically propagating Eq.(1) in imaginary times. The DFT density profile is compared with the MC result for the same system. MC data are obtained by adding to the wave function of the bulk system, described in Ref. [5], a standard Gaussian one-body term with a single variational parameter [12]. The comparison shows a quite good agreement apart near to the surface. This discrepancy is mainly due to the fact that the value of the variational parameter in the one-body term, which is optimized by minimizing the energy per particle, is mainly determined by the higher density region at the center of the trap.

In Fig. 2 we plot the average radius of the trapped gas as a function of the scattering length a . The figure clearly shows that DFT results (squares) converge to a finite radius for $a \gg 1$, while GPE one (dots and dotted line), obtained with $\varepsilon_a(n) = \mathcal{E}_{\text{GPE}}(n, a)$, diverge as $a^{1/5}$ (Thomas-Fermi limit). The convergence to a constant value is expected for the unitary regime, where the properties of the system become universal, i.e. depend only on the density and are insensitive to the actual value of a .

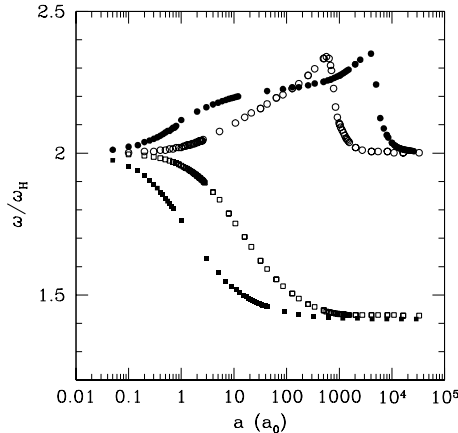


FIG. 3: Monopole (upper curves) and quadrupole (lower curves) frequencies ω as a function of a obtained with DFT. Empty symbols: $N = 500$ bosons; filled symbols: $N = 80000$ bosons.

The oscillation frequencies of both monopole (breathing or compressional) and quadrupole (surface) modes for interacting bosons in harmonic trap can be obtained by numerically solving Eq. (1). The monopole mode is excited by slightly changing the frequency ω_H of the harmonic confinement when computing the initial state $\Psi(\mathbf{r}, t = 0)$, while the quadrupole mode is obtained by using as the initial state $\Psi(\mathbf{r}, t = 0) = e^{i\eta Q}\Psi_0(\mathbf{r})$, where $\Psi_0(\mathbf{r})$ is the ground-state wave function, η is a small parameter and $Q = 2z^2 - x^2 - y^2$ is the standard quadrupole operator. The numerical results are shown in Fig. 3 as a function of a . As the scattering length a is varied, the quadrupole frequency connects smoothly the values [13] $2\omega_H$ appropriate to the non-interacting gas ($a \rightarrow 0$) and $\sqrt{2}\omega_H$ expected in the Thomas-Fermi (TF) regime ($Na/a_H \gg 1$), where $a_H = \sqrt{\hbar/(M\omega_H)}$. As expected, its TF value turns out to be independent of a [13]. The frequency of the monopole mode shows instead a non-monotonous behavior as a function of the scattering length. At small a values (non interacting regime) it recovers the expected $2\omega_H$ limit [13] and in the opposite limit ($a \rightarrow \infty$) it converges to the universal expected unitary value $2\omega_H$ [14]. For intermediate values of a , the breathing frequency should approach the TF value $\sqrt{5}\omega_H$ (independent of a) [13]; but this value is reached only in the $N = 80000$ case, since for $N = 500$ bosons the TF condition $Na/a_H \gg 1$ is satisfied only for a in the unitary regime (as inferred also from the slower convergence to the TF value of the quadrupole frequency).

Finally, we study the effect of three-body losses [15] on the collective oscillations by adding a dissipative term $-i\hbar L_3 n(\mathbf{r}, t)^2 \Psi(\mathbf{r}, t)$ (with $L_3 = 1.1 \cdot 10^{-22}$ cm⁶/sec [3]) in equation (1). In Fig. 4 we report the time evolution of the monopole and quadrupole mean values, $\langle r^2 \rangle$ and $\langle Q \rangle$ respectively, for $N = 80000$ and $a = 10^4 a_0$. During the dynamics the number of atoms (and thus the volume) of the bosonic cloud decreases and, as shown in the figure, $\langle r^2 \rangle$ follows the evolution of the average radius of the ground state with a superimposed oscillation with frequency close to $2\omega_H$. On the contrary the surface mode is only slightly affected by the three-body losses, and $\langle Q \rangle$ oscillates around its starting value with the frequency expected from the chosen value of a .

In conclusion, we have theoretically investigated statics and dynamics of a confined Bose gas by means of a density functional approach which takes into account the whole range of positive scattering lengths from weak-coupling to unitarity. We have shown that the DFT density profiles of the ground state are in good agreement with MC ones. Moreover, by numerically solving the time-dependent density functional equation, we have calculated the frequencies of both monopole and quadrupole modes, analyzing also the effect of three-body losses.

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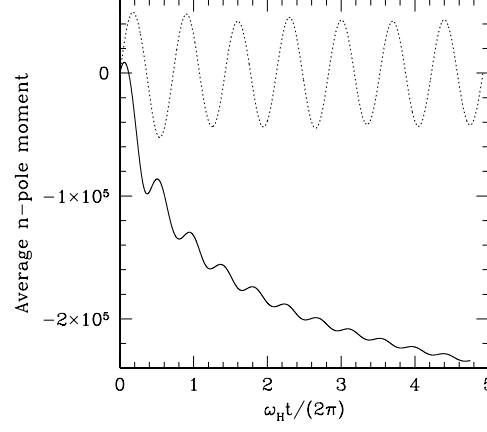


FIG. 4: Time evolution of the average n -pole moment of the trapped Bose gas in the presence of the three-body loss term induced by monopole (solid line) and quadrupole (dotted line) distortions in the $N = 80000$ and $a = 10^4 a_0$ case.

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